Indian J. Phys. **52B**, 379-384 (1978)

Variable-phase approach to electron-hydrogen elastic scattering*.

B. TALUKDAR, D. SENGUPTA AND M. CHATTERJI

Department of Physics, Visva-Bharati University, Santiniketan 731235, *West Bengal*

AND

K. SARKAR AND D. BASU

Indian Association for the Cultivation of Science, Calcutta 700032

(*Received* 28 *November* 1977)

The problem of elastic scattering of an electron off a hydrogen atom is formulated in terms of the variable phase method of Calogero and others. The l-wave phase equation has been derived in the static plus exchange approximation. It has been employed to compute the s-, p- and d-wave phase shifts in the low energy region. The present method appears to represent quite a straight forward approach to the electron-hydrogen phase-shift calculation and is thus expected to supplement the existing sophisticated numerical routines used for this purpose.

1. INTRODUCTION

With the availability of the high speed digital computers it has been possible to solve the equation of the scattering theory to yield accurate predictions of the energy dependence of scattering phase shifts. Typically, in a low-energy electron-atom collision the Schrödinger equation for the scattered electron is obtained by superposing three effects :

(i) the central field interaction between the electron and the nucleus,

(ii) the exchange interaction, and

(iii) the polarization of the atom by the electric field of the incident electron.

The radial Schrödinger equation comes out in the form of a second order linear integro-differential equation. The phase shift determination is accomplished by integrating this equation from the origin to the asymptotic region, where the potential is negligible, and then comparing the phase of the radial wavefunction thus obtained with that of a comparison circular function (Drukerev 1965). In contrast to this approach the present paper will be directed towards the implementation of the variable phase method (VPM) of Calogero and others (Calogero 1967, Ronveanx 1967, Kynch 1952, Levy & Keller 1963, Degasperis 1964, Cox 1965) to study the electron-hydrogen scattering at low energies. In particular, we shall calculate the s-, p- and d-wave scattering phase shifts for wave numbers $k = 0{\cdot}1$ to $1{\cdot}0$ a.u.

* Work supported in part by the Department of Atomic Energy, Government of India.

Traditionally, the VPM proceeds by an ansatz for the wavefunction $f_l(r)$ accompanied by a constraint imposed through the derivative $f_l'(r)$ of the wavefunction. In close analogy to our recent work on the variable phase approach to potential scattering (Talukdar *et al* 1977 cited as paper I hereafter) we derive the phase equation for the electron-hydrogen scattering in the static plus exchange approximation without using the constraint. A brief outline of the derivation has been given in section 2. In section 3 we present the results of s-, p- and d-wave phase shifts computed by using this model and make some observations on such a calculation.

2. Phase Equation

Consider the elastic scattering of an electron by a hydrogen atom. The radial Schrödinger equation for the Scattered electron is given by

$$f_l''(r)+\left[k^2-\frac{l(l+1)}{r^2}\right]f_l(r) = 2\left[V(r)f_l(r)+\int_0^\infty W_l(s,r)f_l(s)ds\right], \quad \ldots (1)$$

where k = the wave number of the scattered electron and

$$V(r) = -e^{-2r}\left(2+\frac{1}{r}\right). \quad \ldots (2)$$

The prime or f_l denotes differentiation with respect to r. In this paper we shall use atomic units throughout. The exchange operator is represented as

$$W_l(s,r) = \pm 4rse^{-(s+r)}[\gamma_l(r,s)/(2l+1)-\tfrac{1}{2}(k^2+1)\delta_{l0}] \quad \ldots (3)$$

with

$$\gamma_l(r,s) = \begin{cases} \dfrac{s^l}{r^{l+1}} & , \ r \geqslant s \\ \dfrac{r^l}{s^{l+1}} & , \ s \geqslant r \end{cases} \quad \ldots (4)$$

and δ_{l0}, the Kronecker delta.

The signs $\pm$ in eq. (3) refer to the singlet and triplet scattering. Treating the right hand side of eq. (1) as an inhomogeneity term and using the Green's function of paper 1 the solution of eq. (1) can be written in the form

$$f_l(r) = \xi_l(r)[\cos\delta_l(r)\hat{j}_l(kr)+\sin\delta_l(r)\hat{\eta}_l(kr)] \quad \ldots (5)$$

where

$$\xi_l(r)\cos\delta_l(r) = C_l(r) = 1-\frac{2}{k}\int_0^r dr\hat{\eta}_l(kr')[V(r')f_l(r')+\int_0^\infty W_l(s,r)f_l(s)ds] \quad \ldots (6a)$$

and

$$\xi_l(r)\sin\delta_l(r) = S_l(r) = -\frac{2}{k}\int_0^r dr\hat{j}_l(kr)[V(r')f_l(r')+\int_0^\infty W_l(s,r')f_l(s)ds]. \quad \ldots \quad (6b)$$

In eq. (5) $\delta_l(r)$ represents the phase function and $\xi_l(r)$, the amplitude function. Note that the two functions $C_l(r)$ and $S_l(r)$ tend towards finite limits as $r \to \infty$ because both the local and exchange potentials, in the asymptotic limit, go to zero faster than $1/r$. In the variable phase method the phase shift defined by

$$\tan\delta_l = \lim_{r\to\infty}\tan\delta_l(r) = \frac{S(\infty)}{C(\infty)}. \quad \ldots \quad (7)$$

The derivation of the amplitude and phase equations may now be facilitated by using the technique developed in paper 1.

The phase equation is given by

$$\delta^l(r) = -\frac{2}{k}[\hat{j}_l(kr)\cos\delta_l(r)-\hat{\eta}_l(kr)\sin\delta_l(r)]^2\times$$

$$\times\Big[V(r)+\int_0^\infty W_l(s,r)\exp\Big\{-k\int_0^r\Big(\frac{\hat{j}_l(kt)\cos\delta_l(t)-\hat{\eta}_l(kt)\sin\delta_l(t)}{\hat{j}_l(kt)\cos\delta_l(t)-\hat{\eta}_l(kt)\sin\delta_l(t)}\Big)\times dt\Big\}\Big] \quad \ldots \quad (8)$$

Thus the phase equation for the electron-hydrogen elastic scattering is a simple first order non-linear differential equation with the initial condition $\delta(0) = 0$. We have carried out the numerical integration of eq. (8) by the method of successive approximation owing to the presence of the infinite integral on the right hand side. In the static approximation the phase equation takes the form.

$$\delta_l'(r) = -\frac{2}{k}V(r)[\hat{j}_l(kr)\cos\delta_l(r)-\hat{\eta}_l(kr)\sin\delta_l(r)]^2 \quad \ldots \quad (9)$$

We have solved eq. (9) by a stepwise integration method using the Runge-Kutta algorithm with an appropriate stability check (Scarborough 1971, Seckett & Hurt 1967). The integration has been carried out until $\delta_l(r)$ remains stationary with r. These values of $\delta_l(r)$ are then used for starting the iteration to obtain the phase shift in the static plus exchange approximation. We have found that only five to six iterations are necessary.

3. Results and Discussion

Table 1 illustrates the results of our phase shift calculation at wave numbers varying from 0·1 to 1·0 a.u. In this table we have included our results for the static phase shifts as well as those for singlet (δ_l^+) and triplet (δ_l^-) scattering. The computed values of δ_l are in agreement with those obtained by numerical integration (Mott & Massey 1965, John 1960) of the scattering equation upto 3 to 4 significant digits. We have, therefore, not included the latter numbers in the table.

Table 1. Electron-hydrogen elastic phase shifts (rad) for s-, p- and d-waves.

Wave number	s-wave			p-wave			d-wave		
k	δ_0	δ_0^+	δ_0^-	δ_1	δ_1^+	δ_1^-	δ_2	δ_2^+	δ_2^-
0·1	0·7211	2·3961	2·9080	0·0003	−0·0012	0·0021			
0·2	0·9730	1·8710	2·6790	0·0021	−0·0084	0·0166			
0·3	1·0462	1·5080	2·4613	0·0071	−0·0261	0·0502	0·0002	−0·0006	0·0009
0·4	1·0570	1·2391	2·2572	0·0146	−0·0439	0·1000	0·0007	−0·0020	0·0027
0·5	1·0450	1·0312	2·0705	0·0260	−0·0702	0·1693	0·0014	−0·0039	0·0070
0·6	1·0210	0·8691	1·9010	0·0447	−0·0870	0·2374	0·0032	−0·0062	0·0146
0·7	0·9934	0·7440	1·7491	0·0580	−0·1077	0·2792	0·0052	−0·0103	0·0227
0·8	0·9630	0·6510	1·6140	0·0750	−0·1092	0·3126	0·0086	−0·0125	0·0339
0·9	0·9360	0·5890	1·5012	0·0927	−0·1149	0·3486	0·0128	−0·0150	0·0447
1·0	0·9056	0·5427	1·3910	0·1115	−0·1058	0·3580	0·0176	−0·0174	0·0555

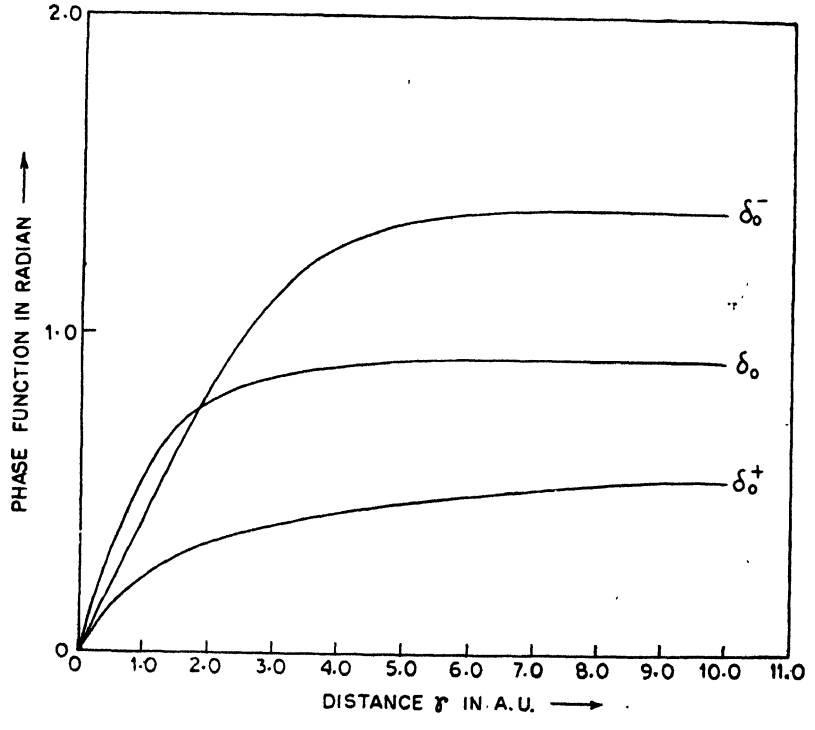

Fig. 1. Variation of the s-wave phase functions with the radial distance r.

The behaviour of the phase functions with increasing radial distance is shown in figures 1 and 2. The s-wave phase functions are included in figure 1. On the other hand, in figure 2 we have plotted the p- and d-wave phase functions. To facilitate comparison of the effects of different regions of the potential in producing phase shifts, all the curves are drawn for $k = 1{\cdot}0$ a.u. Looking closely into these figures we see that the dominant contribution to the s-wave phase shifts is made by the region of the potential with small r values. While the important contribution to the p- and d-wave phase shifts comes from relatively large r values. It thus appears that the VPM may be used to substantiate the general statement that the region of the space sampled by the scattering lies at larger r for greater l.

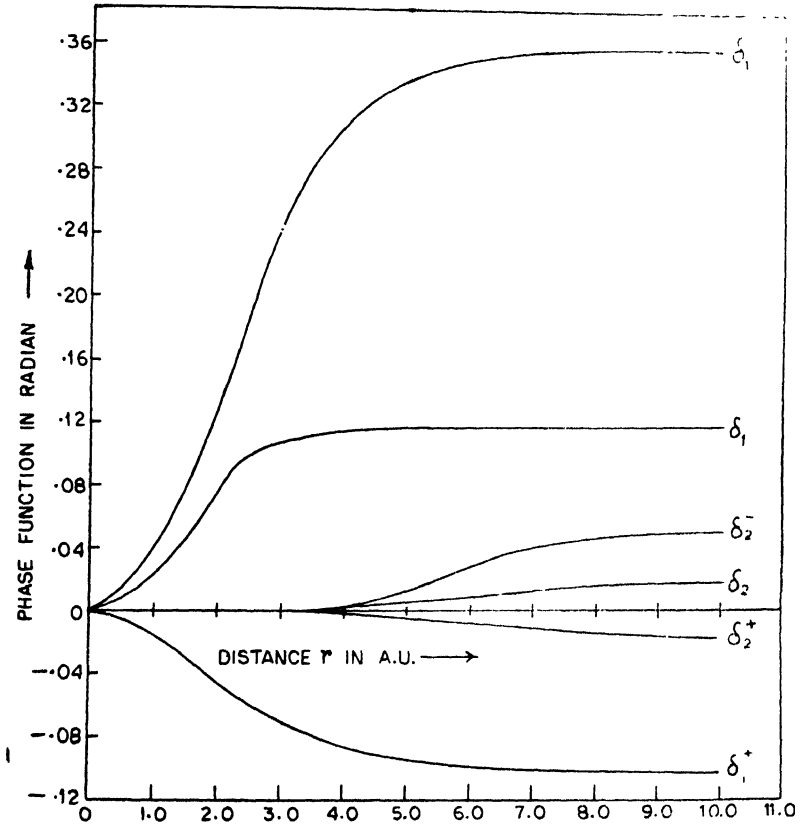

Fig. 2. Variation of the p- and d-wave phase functions with r.

Working within the framework of the present model we have obtained quite encouraging results. This seems to indicate that it may be possible to construct new algorithms for the exact calculation of various electron-atom scattering parameters (phase shift, scattering length etc.) based on the variable

phase method. For example, introduction of the close coupling approximation and the effect of the polarization potential will be the next logical steps enabling one to make a more detailed investigation.

Acknowledgment

One of the authors (MC) is graetful to the University Grants Commission,. Governments of India, for a research grant.

References

Beckett R. & Hurt J. 1967 *Numerical Calculations and Algorithms* (McGraw Hill, New York).

Calogero F. 1967 *Mathematics in Science and Engineering* Vol. **35** (Academic, New York).

Cox J. R. 1965 *Nuovo Cimento* **37**, 474.

Drukerev G. F. 1965 *The Theory of Electron-Atom Collision* (Transl. S. Chomet, Academic, New York).

Degasperis A. 1964 *Nuovo Cimento* **33** 939.

John T. L. 1960 *Proc. Phys. Soc. (London)* **76**, 532.

Kynch G. J. 1952 *Proc. Phys. Soc.* **65A**, 83, 94.

Levy S. R. & Keller J. B. 1963 *J. Math. Phys.* **4**, 54.

Mott N. F. & Massey H. S. W. 1965 *The Theory of Atomic Collissions* (Oxford, Clarandon Press).

Renveanx A. 1969 *Am. J. Phys.* **37**, 135.

Scarborough J. B. 1971 *Numerical Mathematical Analysis* (Oxford and I. B. H. Pub. Co., Calcutta).

Talukdar B., Chatterji D. & Banerji P. 1977 *J. Phys.* (to be published), cited as paper I.